Leadership Class Configuration Interaction (LCCI) Code
Project of SciDAC/UNEDF

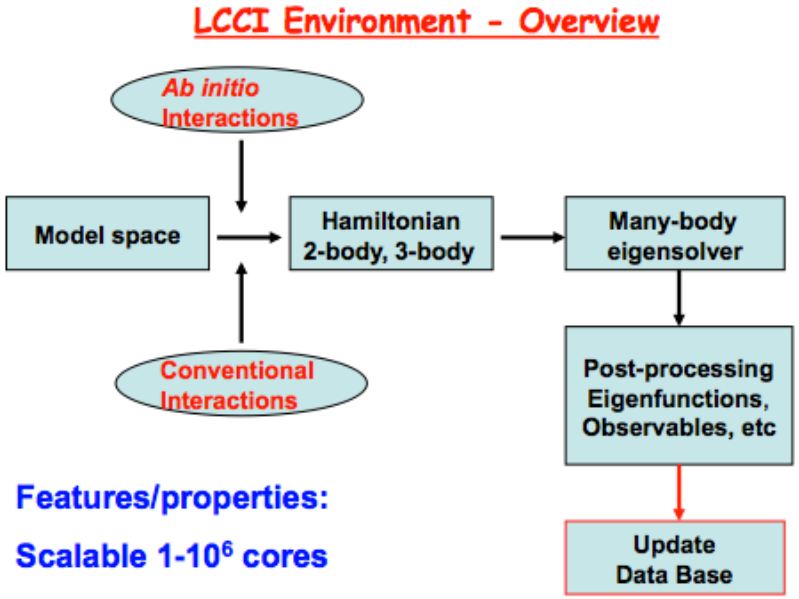
Introduction

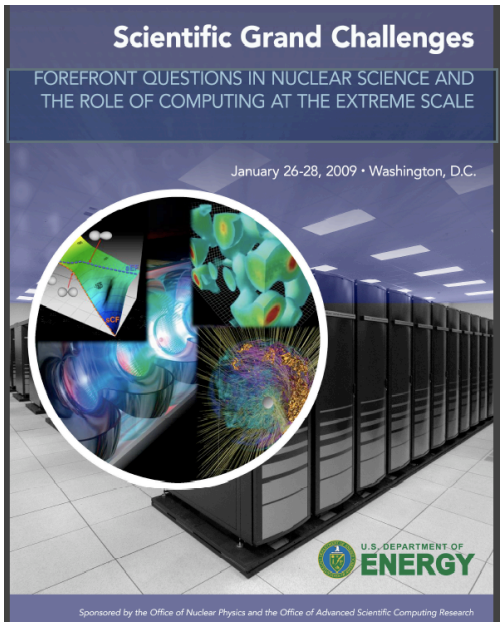
James P. Vary
Iowa State University
jvary@iastate.edu

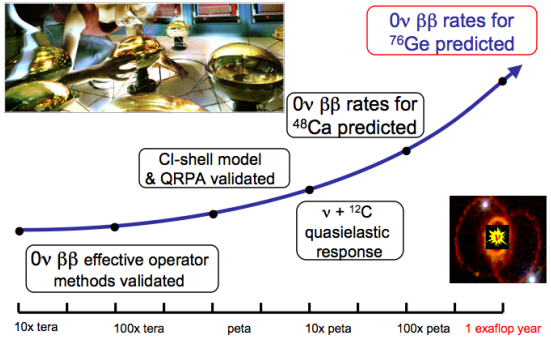
Version 6.5- October 27, 2011

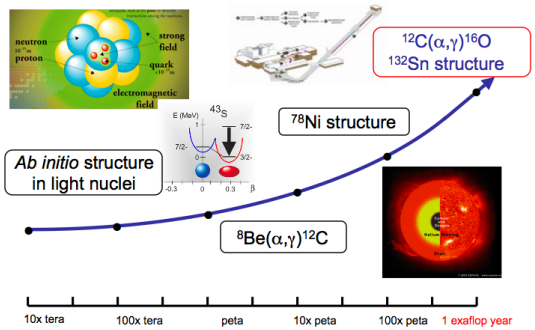
Leadership Class Configuration Interaction (LCCI) Environment: *ab initio* computational nuclear physics resources for the future

- SciDAC/UNEDF initiative to unify, preserve and disseminate valuable CI codes & resources
- User-friendly environment for researchers to download and run state-of-the-art CI codes
- Archives results (e.g. wavefunctions, densities,…) from large-scale production runs
- Aims to enable CI calculations planned for extreme-scale computers and archive the results

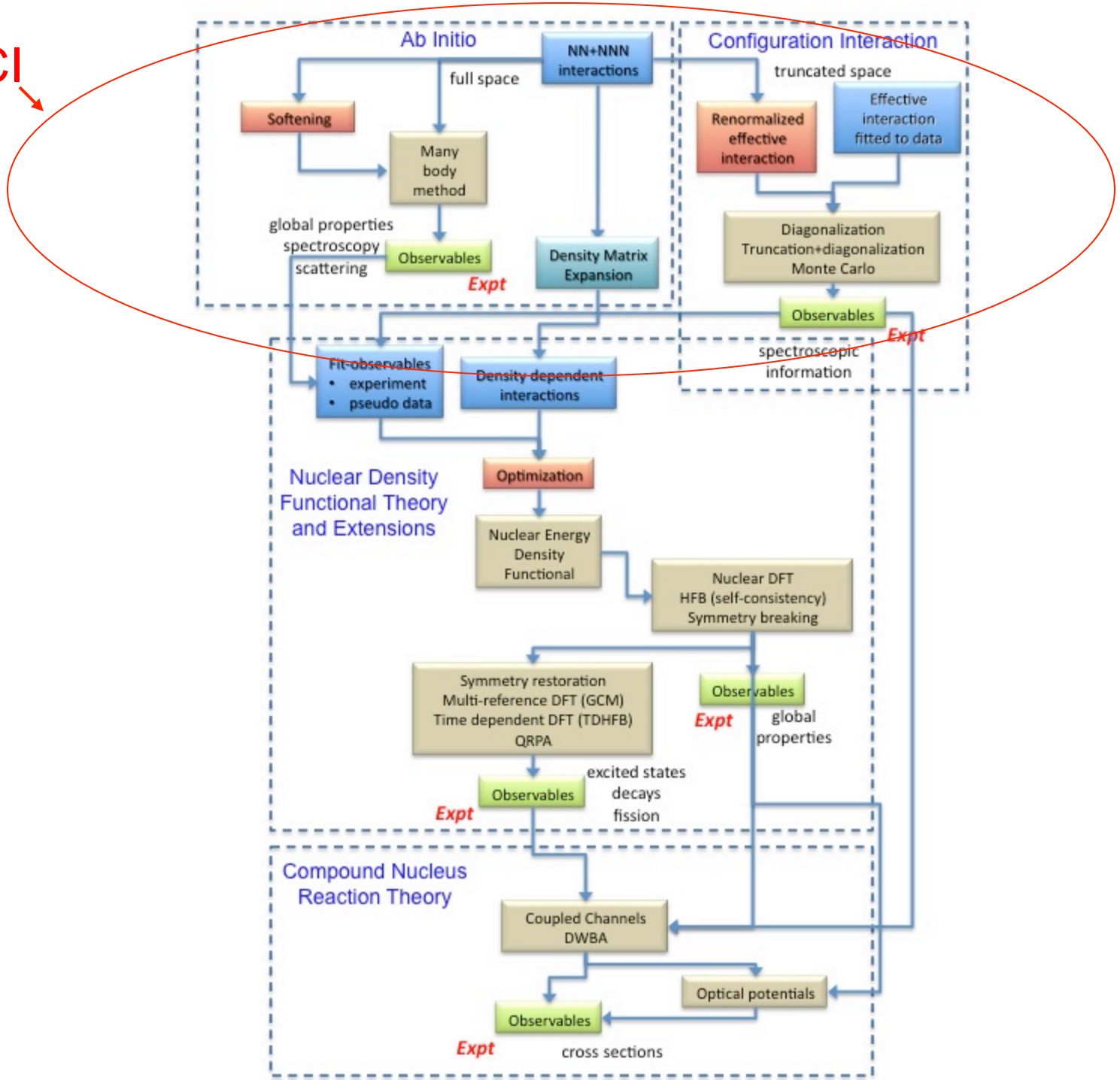








LCCI


Ab Initio
NN+NNN interactions
full space
Softening
Many body method
global properties
spectroscopy
scattering
Observables
Expt
Density Matrix Expansion
Configuration Interaction
truncated space
Renormalized effective interaction
Effective interaction fitted to data
Diagonalization
Truncation+diagonalization
Monte Carlo
Observables
Expt
spectroscopic information
Fit-observables
• experiment
• pseudo data
Density dependent interactions
Optimization
Nuclear Density Functional Theory and Extensions
Nuclear Energy Density Functional
Nuclear DFT
HFB (self-consistency)
Symmetry breaking
Symmetry restoration
Multi-reference DFT (GCM)
Time dependent DFT (TDHFB)
QRPA
Observables
Expt
global properties
Observables
excited states
decays
fission
Expt
Compound Nucleus Reaction Theory
Coupled Channels
DWBA
Optical potentials
Observables
Expt
cross sections

LCCI codes/scripts
initial deposits October 2009

Codes/Scripts	Contact	email	Updated	Final update
BIGSTICK	Calvin Johnson	cjohnson@sciences.sdsu.edu	June 2011	Nov 2011
MFDn	Pieter Maris	pmaris@iastate.edu	Sept 2011	Nov 2011
NuShellX	Mihai Horoi	horoi@phy.cmich.edu	March 2011	Nov 2011
	Eric McDonald	em@msu.edu		
trdens	Petr Navratil	navratil@triumf.ca	April 2010	Nov 2011
ncsmv2eff	Petr Navratil	navratil@triumf.ca	March 2010	Nov 2011
LCCI-wrapper	Maris/Johnson	pmaris@iastate.edu	July 2011	Nov 2011

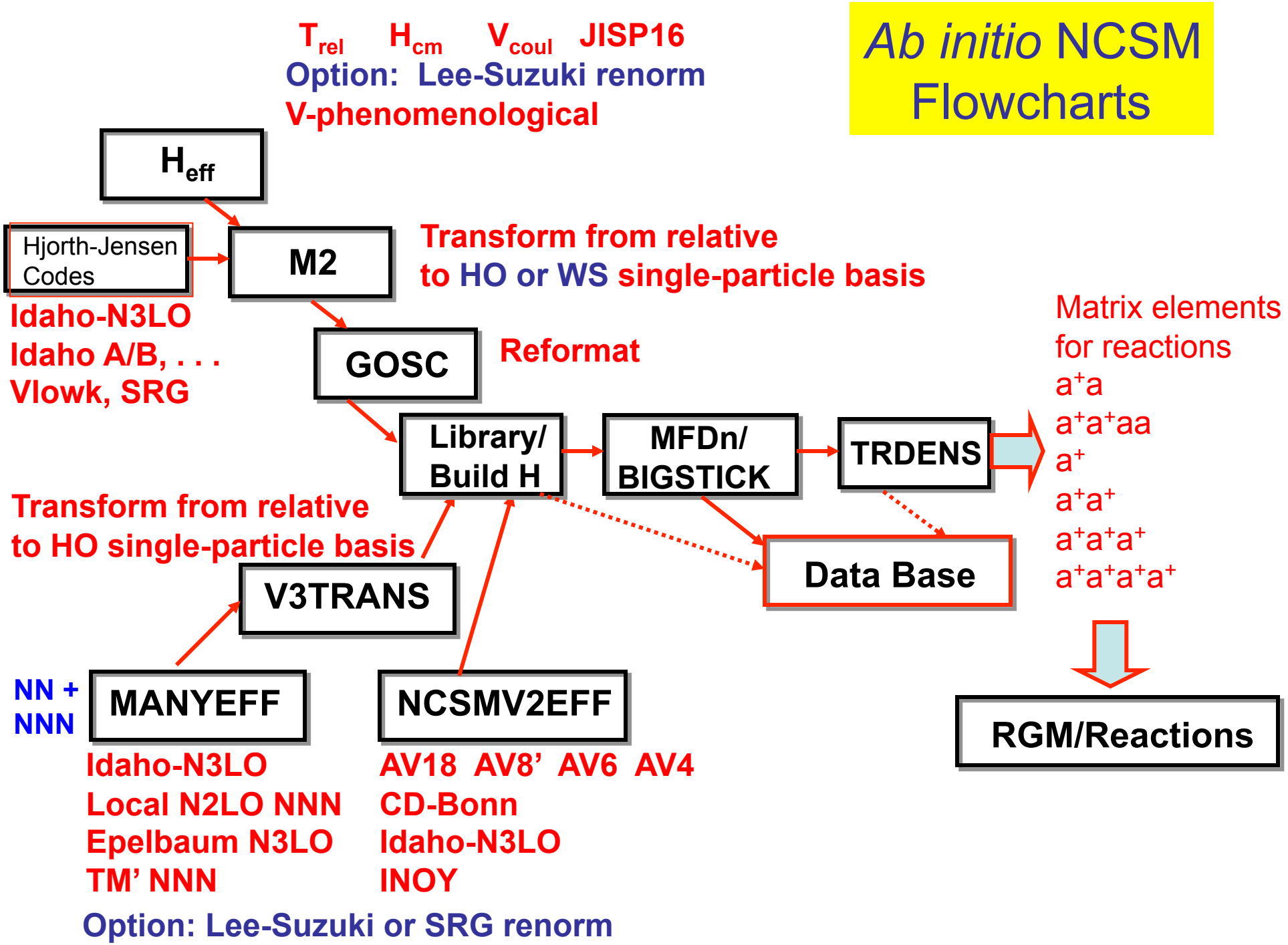
Source codes for each resides in its own subdirectory in NERSC project space:

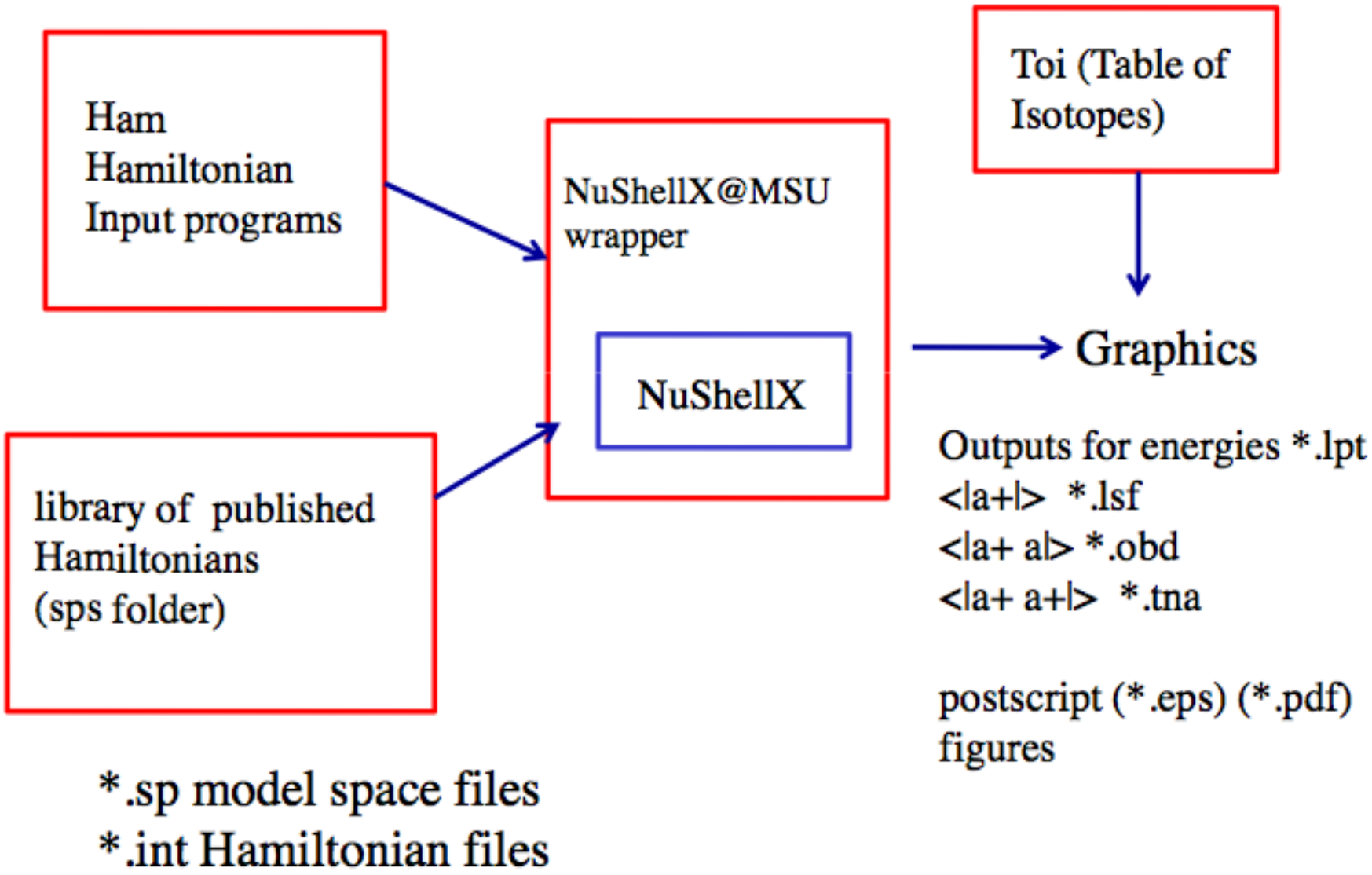
/project/projectdirs/unedf/lcci

with a README file, one or more scripts, and test cases.

In addition, this introduction and an introduction to the DBMS reside there and are updated as major developments warrant.

Ab initio NCSM Flowcharts




Ham
Hamiltonian
Input programs
Toi (Table of Isotopes)
NuShellX@MSU
wrapper
NuShellX
Graphics
library of published
Hamiltonians
(sps folder)
Outputs for energies *.lpt
<|a+|> *.lsf
<|a+ a|> *.obd
<|a+ a+|> *.tna
postscript (*.eps) (*.pdf)
figures
*.sp model space files
*.int Hamiltonian files

BIGSTICK – a configuration-interaction code:

W. E. Ormand, LLNL; C. W. Johnson, SDSU; P. G. Krastev, SDSU

- **Purpose**: Solve the general many-fermion problem.
- **Method**: Lanczos algorithm to find low-lying eigensolutions of large Hamiltonian matrix; on-the-fly matrix-vector multiply using factorization.
- **Input**: General single-fermion basis, assuming good angular momentum *j*.
  - User-friendly interactive input.
  - Two "species" of particles, e.g. proton/neutron (half-integer *j*) or spin up/down (integer *j*); allows general radial wavefunctions.
  - Flexible truncation of many-body basis covering many common choices.
  - General two-body interactions, assuming only rotational invariance, read in as files of precomputed matrix elements; can read in different formats and multiple files.
  - Can assume or break isospin symmetry.
  - General three-body interactions
- **Output:** Produces output wavefunctions compatible with TRDENS.
  - Option to automatically compute one-body transitions densities without further post-processing.
- **Implementation:** M-scheme many-body basis; states of good *J* automatically recovered.
  - Works well both on serial machines and with MPI parallelization.
  - Hybrid MPI/OpenMP parallelization.

For more info see README file at:
/project/projectdirs/unedf/lcci/BIGSTICK

NuShellX – a configuration-interaction code:

B. A. Brown, E. McDonald, M. Horoi, W. D. M. Rae

•**Purpose**: Solve the general many-fermion problem.

•**Method**: Lanczos algorithm to find low-lying eigensolutions of large Hamiltonian matrix; on-the-fly matrix-vector multiply.

•**Input**: General single-fermion basis, assuming good angular momentum *j*.

- User-friendly interactive input.
- Two "species" of particles, e.g. proton/neutron
- Flexible truncation of many-body basis covering many common choices.
- General two-body interactions, assuming only rotational invariance, read in as files of precomputed matrix elements; can read in different formats and multiple files.
- Can assume or break isospin symmetry.

• **Output:** Produces wavefunctions, spectroscopic factors, one-body transition densities

• **Implementation:** J-scheme many-body basis

- Works well both on serial machines and with OpenMP parallelization.
- Hybrid MPI/OpenMP parallelization (completed/testing in prgress).
- Wrapper codes for Table of Isotopes and Hamiltonians

For more info see README file at:
/project/projectdirs/unedf/lcci/nushellx

MFDn - Many Fermion Dynamics - nuclear
A configuration interaction code

- General-purpose and portable many-fermion code; solves very large matrix Hamiltonian in a Slater determinant basis
- Uses general single-fermion basis, assuming good angular momentum *j*.
- One or two "species" of particles, e.g. proton/neutron (half-integer *j*); allows general radial wavefunctions
- Flexible truncation of many-body basis covering several common choices.
- General two-body and three-body interactions, assuming only rotational invariance; read in as files of precomputed matrix elements; can read in different formats; reads in and independently scales multiple interaction files
- Option to run with an external field
- M-scheme many-body basis; states of good *J* automatically recovered.
- Lanczos eigensolver using full many-body matrix stored in core.
- Works both on serial machines and with MPI/OpenMP parallelization
- Produces output wavefunctions compatible with TRDENS
- Option to automatically compute one-body transition densities without further post-processing
- Options to evaluate various suites of observables
- Total J version (in progress)

For more info see README file at:
/project/projectdirs/unedf/lcci/MFDn

TRDENS basic features

- **Purpose**: Calculate matrix elements of combinations of creation and annihilation operators
  - Currently coded: $\langle a^+a\rangle, \langle a^+a^+aa\rangle, \langle a^+\rangle, \langle a\rangle, \langle a^+a^+\rangle, \langle aa\rangle, \langle a^+a^+a^+\rangle, \langle aaa\rangle, \langle a^+a^+a^+a^+\rangle, \langle aaaa\rangle, \langle a^+a^+a\rangle \ldots$
- Initial and final eigenstates from the same nucleus or from different nuclei
  - Eigenstates declared as pointers: For the same nucleus $|f\rangle \Rightarrow |i\rangle$
  - Currently eigenstates generated by the following codes can be input
    - "Arizona" MFD
    - NCSD (No-Core in Slater Determinant basis)
      - calculates on the fly with hashing search
    - Antoine
    - Robert Roth's Importance-Truncated NCSM code
    - MFDn - v13
    - Bigstick
- Output
  - ASCII file with the densities
  - Observables such as B(E2), B(M1), B(GT), translationally-invariant densities, form factors, mean values of H, T, Coulomb…

For more info see README file at:
/project/projectdirs/unedf/lcci/trdens

Overview of Iowa State "upstream" codes

Further information: James Vary (jvary@iastate.edu)

Heff

Generates two-body matrix elements of an NN interaction in the relative coordinate harmonic oscillator basis. Includes capability to unitarily transform from one harmonic oscillator basis to another. Contains the option to perform the Lee-Suzuki renormalization transformation.

M2

Transforms two-body matrix elements from the relative coordinate harmonic oscillator basis to the harmonic oscillator single particle basis (Talmi-Moshinsky Transformation). Also contains the option to transform to the Woods-Saxon single particle basis by a finite expansion in an underlying harmonic oscillator basis. Options include capability of generating Trel, Vcoul, etc matrix elements in the chosen single particle basis. Option to generate Minnesota and other interactions.

GOSC

Transforms output files from M2 (matrix elements grouped by [J,T,Parity]) to one of the input formats used by MFDn (e.g. matrix elements grouped by [a,b,c,d]). The output format of GOSC is specified by the parameter "IPOTENTIAL" within the code.

LCCI Wrapper

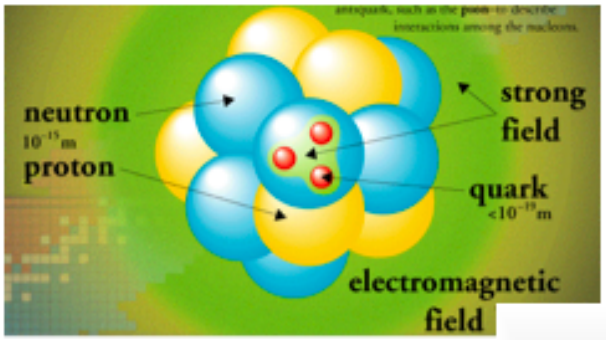
Goal: Single LCCI wrapper to access all LCCI resources

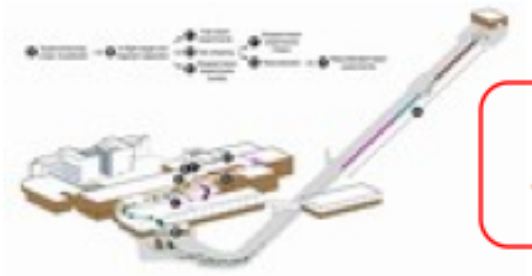
Initial working wrappers - BIGSTICK, MFDn, NuShellX

LCCI python wrapper development stages
Intermediate - BIGSTICK/MFDn (Year 4)
Final - BIGSTICK/MFDn/NuShellX (Year 5)

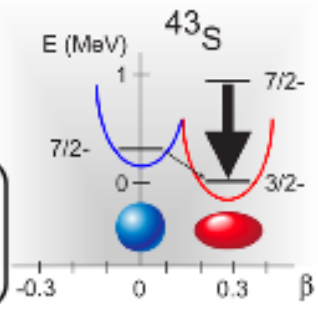
MFDn: - sets up a run for Franklin or Hopper using an available
2- or 3-body interaction files
- Python script generates a batchscript to be submitted to batch queue
- successful run produces output suitable for inclusion in LCCI database

BIGSTICK: - menu driven input already, user friendly
- template input files available
- template batchscript for submission to batch queue available



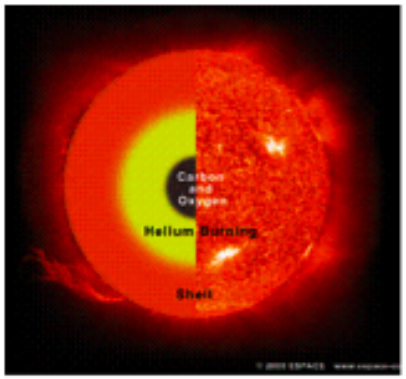


$^{12}C(\alpha,\gamma)^{16}O$
^{132}Sn structure



^{78}Ni structure

Ab initio structure
in light nuclei

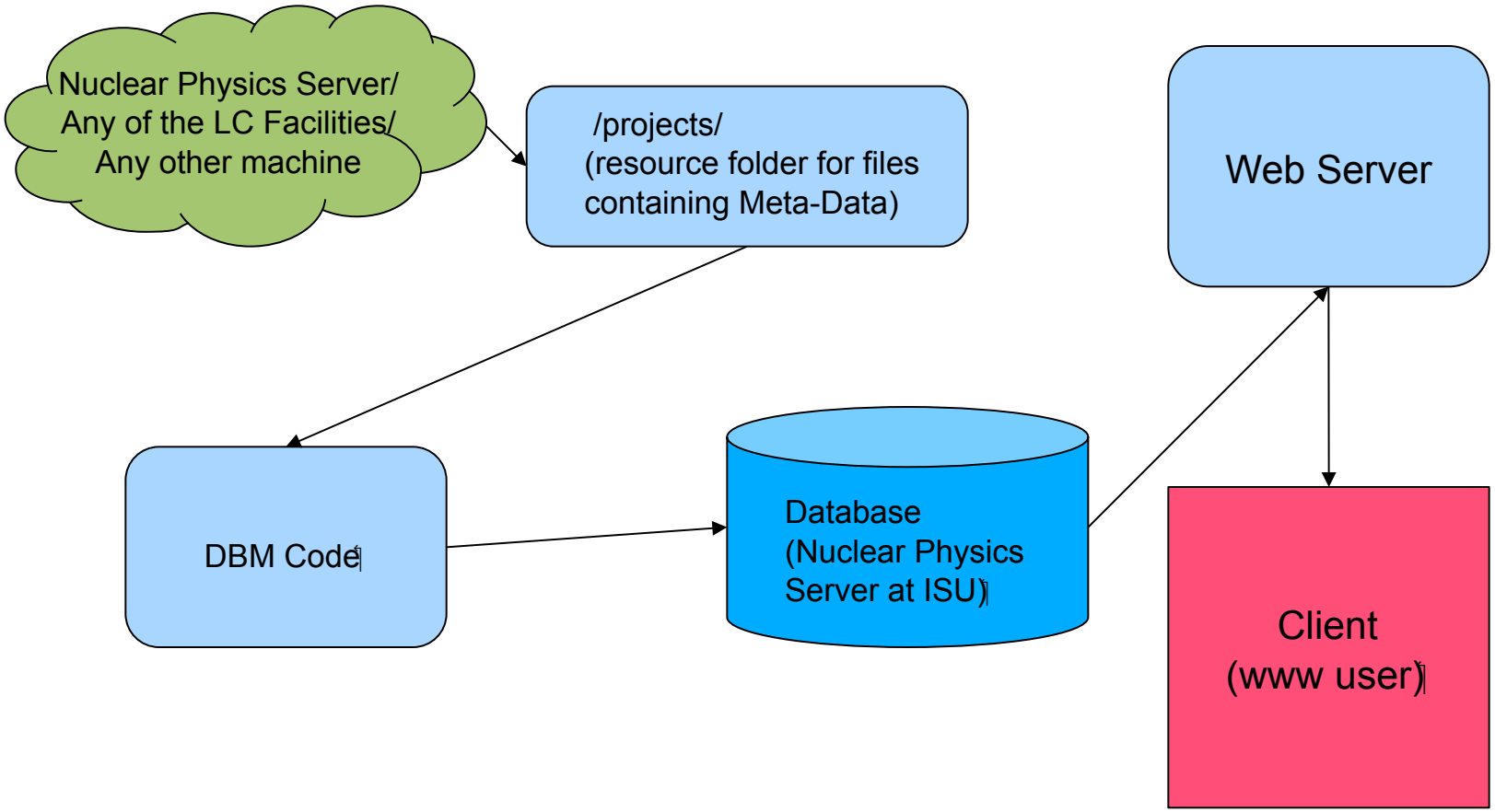


$^{8}Be(\alpha,\gamma)^{12}C$

10x tera | 100x tera | peta | 10x peta | 100x peta | 1 exaflop year

DOE Workshop on Forefront Questions in Nuclear Science
and the Role of High Performance Computing,
Gaithersburg, MD, January 26-28, 2009

Data Base Management System
Current Prototype



Nuclear Calculations DBMS

A Database Indexing Previously-Calculated, Archived Nuclei

DBMS Home | List All | Search

Summary of Available Calculations

2 Body Potential: *Any* JISP16 JISP2010 Minnesota N3LO N3LO3NF

3 Body Potential: *Any* N3LO3NF NONE

External Field: Any

User: Any

Number of Protons ↑ / Number of Neutrons →

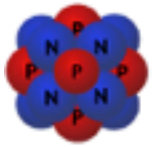
Protons \ Neutrons	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
10									14														
9										38													
8									12		26												
7																							
6				4			26	21															
5																							
4			22	19	21	21	23	9	12	8	4												
3				33	15	13	4																
2		35	71	3	14	3	25	2	2														
1		2																					
0				21	45	10	30	16	69	25	32	3	16	9	24	8	11	8	5	9	42	8	11

Protons \ Neutrons	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44
10																						
9																						
8																						
7																						
6																						
5																						
4																						
3																						
2																						
1																						
0		7		3		2		2		3		2		4		5	6	3	4	5		2

6828 calculations in 958 runs of 63 distinct nuclei.

http://nuclear.physics.iastate.edu/info/

Sample data base entry for single run with pull-downs for details



Nuclear Calculations DBMS

A Database Indexing Previously-Calculated, Archived Nuclei

12
C
6 6
Carbon

Number of states calculated: 15
Initial state for transitions: #1

Potentials
2 Body: N3LO3NF
3 Body: N3LO3NF

External Field: NONE
Parity: positive (+)
m_j: 0

Nmax: 4
Nshell
Z: from 1 to 6
N: from 1 to 6

Additional Quantities Calculated

- J – Total Angular Momentum
- T – Isospin
- radii – RMS Radii
- H_{cm} – Energy of the Center of Mass
- obdme – One Body Density Matrix Elements

▾ Execution Details

User@Machine: James P. Vary @ NERSC-franklin (JobID: 7255816.nid00003)
Working Folder: /global/homes/u/u16347/demo7
Running Time: 00:05:18 (Started: 2011-07-25 11:51:33; Ended: 2011-07-25 11:56:51).

▸ General Data Files

▸ E,J,T,radii,Hcm - Result Files

▸ OBDME - One Body Density Matrix Elements Files

▸ Hamiltonian Directories

pull-downs for details

LCCI Meeting March 17-19, 2011

Issues discussed:

Progress on code & script developments

Update schedules (slide 5)

Modifications to Year 5 goals, deliverables (slide 25)

What to propose for SciDAC-3

Some specific questions discussed:

LCCI thrust areas to propose for SciDAC3:

- double beta decay (slides 16, 18)
- ab-initio nuclear reactions (slides 16, 19)
- structure of medium mass nuclei: 78Ni, 132Sn (slides 16, 19)

If/how to fold the upstream codes into wrapper -> SciDAC3

Will additional researchers deposit .info files to DBMS -> Yes

Desired features for DBMS/Workflow and their priorities -> Ongoing

What happens to UNEDF web site & m308 at end of UNEDF?

-> UNEDF Council to address

Making the LCCI repository public, e.g. via UNEDF web site,
or via FRIB or via NNDC -> possibly all 3

Outcomes reflected in updated version of LCCI Introduction available for downloading from NERSC:
/project/projectdirs/unedf/lcci/LCCI_Introduction_v6.3.pdf

"Proton-Dripping Fluorine-14"

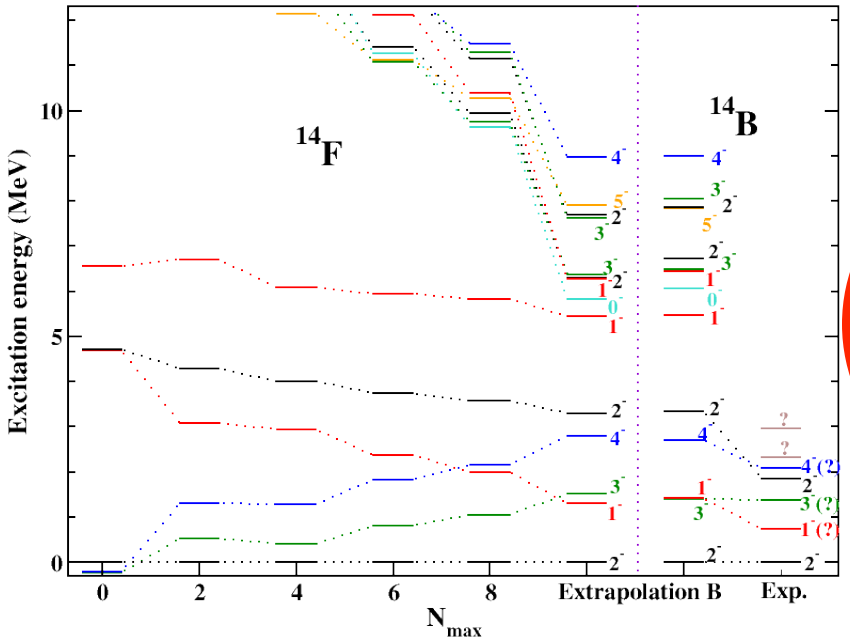
Objectives

- Apply *ab initio* microscopic nuclear theory's predictive power to major test case

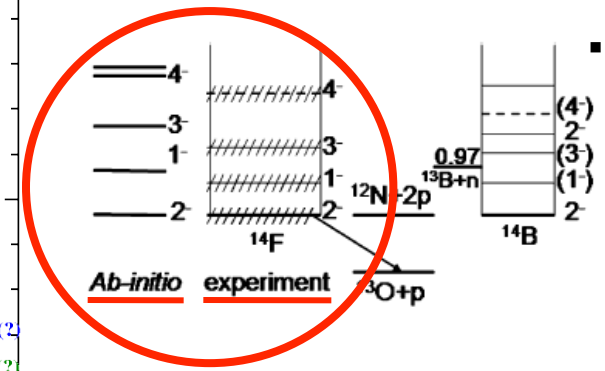
Impact

- Deliver robust predictions important for improved energy sources
- Provide important guidance for DOE-supported experiments
- Compare with new experiment to improve theory of strong interactions

P. Maris, A. Shirokov and J.P. Vary,
Phys. Rev. C 81 (2010) 021301(R)



Experiment confirms our published predictions!



V.Z. Goldberg et al.,
Phys. Lett. B 692, 307 (2010)

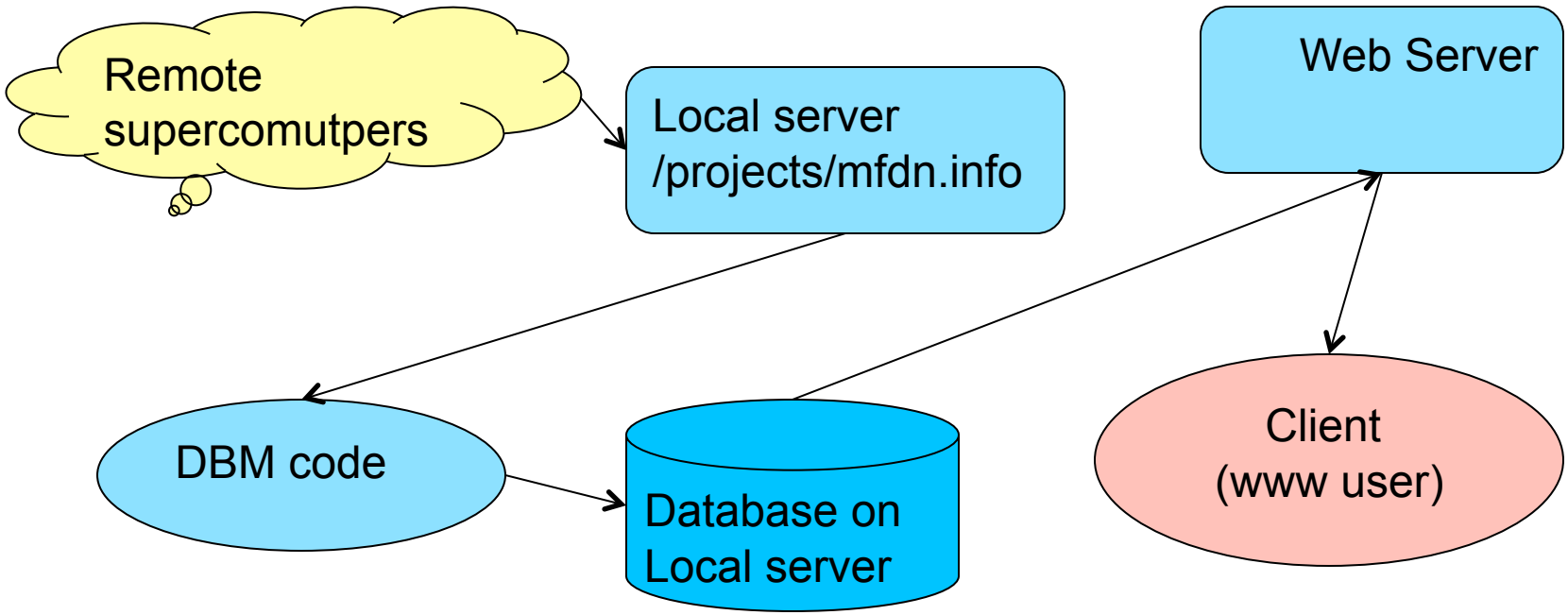
- Dimension of matrix solved for 14 lowest states ~ 2×10^9
- Solution takes ~ 2.5 hours on 30,000 cores (Cray XT4 Jaguar at ORNL)
- "Scaling of ab-initio nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97 (2010)

U.S. DEPARTMENT OF ENERGY | Office of Science

INCITE Advancing America's Science and Industrial Competitiveness

UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

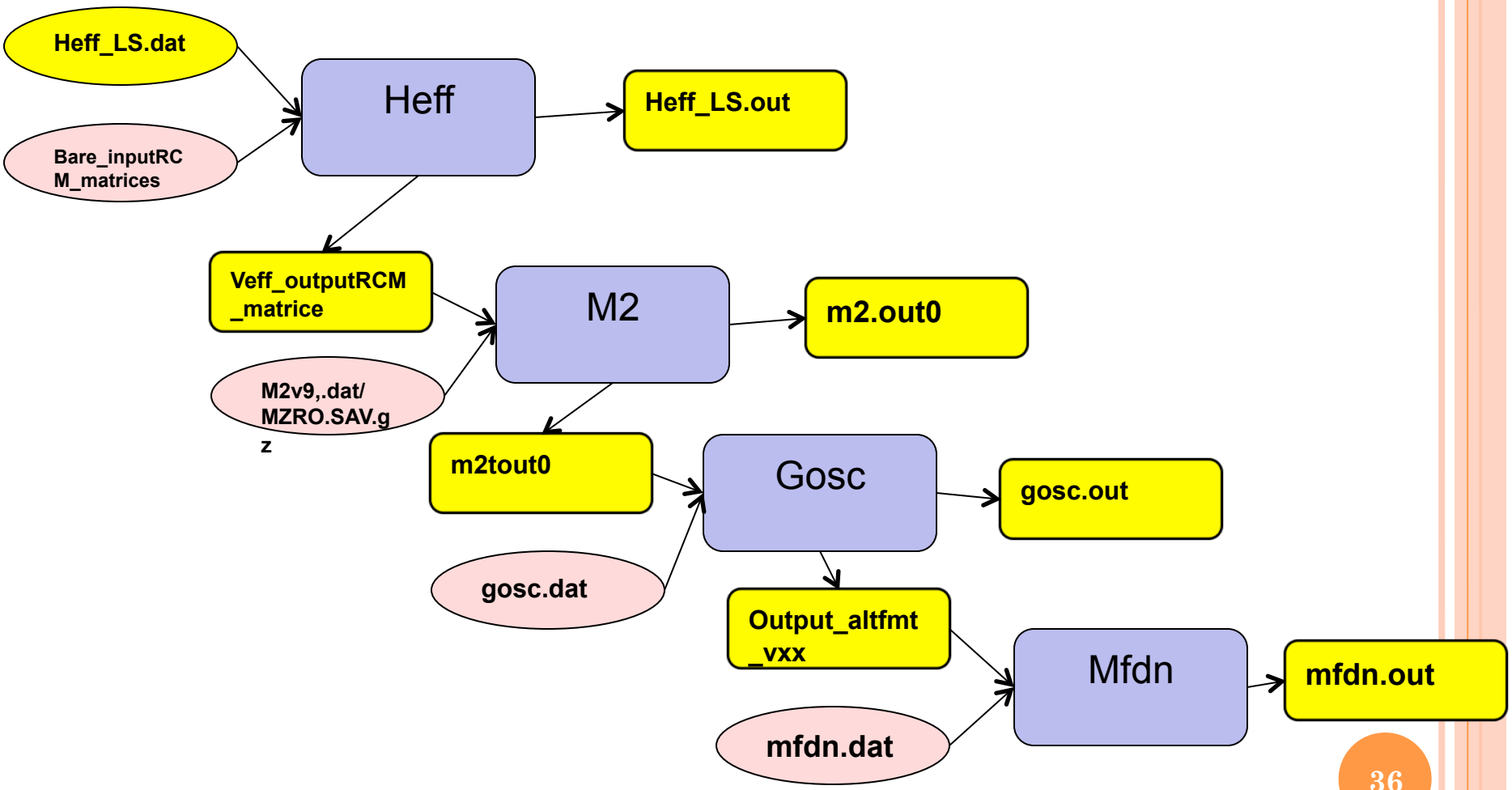
Data Base Management System
System Design and Components



1. DB Manager: parses the mfdn.info file and inserts the run record to Database
2. Web based front end: searches and lists existing runs
3. DB Server: stores all the related metadata for each of MFDn run

F. Liu and M. Sosonkina, Ames Lab

Detailed data flow between components



NAVIGATION

- Home
- My Files
- My Account
- List of All Files
- Nuclear Physics Calculator
- Many Fermion Dynamics
- Other Resources
- MFDn DBMS

QUOTE

The Cosmos is all that is or ever was or ever will be. Our feeblest contemplations of the Cosmos stir us there is a tingling in the spine, a catch in the voice, a faint sensation, as if a distant memory, of falling from a height. We know we are approaching the greatest of mysteries.

~Carl Sagan

Nuclear Physics Calculator

http://nuclear.physics.iastate.edu

The "nuclear physics calculator: extreme single-particle shell model" was written by Dr. James P. Vary. For details on how to use the calculator and on it's function, see SS#1, SS#2, and SS#3.

Quick how-to: change the settings as you desire, then click "calculate". The calculation will run and the results will be returned to you as a text file momentarily.

Basic Settings:

Protons: 79 Neutrons: 118

Coulomb of uniform charged sphere:

- (•) no (solve for neutrons)
- ( ) yes (solve for protons)

Advanced Settings:

Max principal quantum number of HO basis (*n*) [0 - 20]: 12

Max orbital angular momentum (*l*) [0 - 10]: 7

h-bar*Ω of HO basis in MeV: 7.000

Gauss points for numeric integration [mult of 8, up to 136]: 48

Output Settings:

Return: Saxon-Woods wave functions only.

Number of r-points on uniform grid [200-1000]: 600

Grid size in fm [0.01 - 0.25]: 0.05

Perey & Perey *Modified* Parameters (defaults are normally okay):

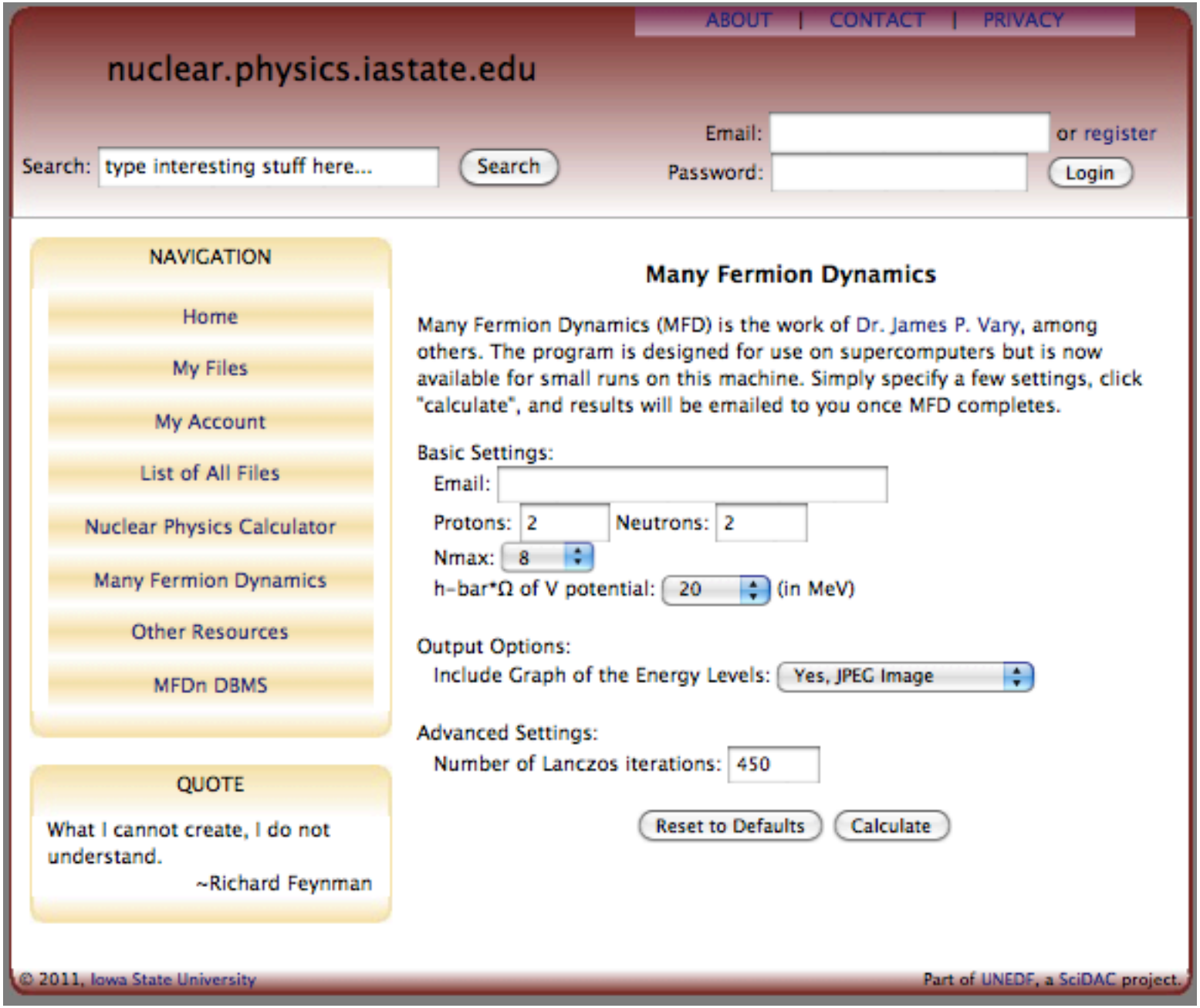
	Central Potential	Spin-Orbit Potential
Well Depth [MeV]	-47.9548215720859	15.0
X x $A^{1/3}$ for radius [fm]	1.25	1.25
Diffuseness [fm]	0.65	0.47

☑ Auto-solve for Central Potential Well Depth

Reset to Defaults | Calculate

Downloads text file of results to you computer: spectra, wavefunctions, & densities

Realistic nuclear structure calculations online
Delivers text file and (optional) graph via email



For discussion
DNP – Fall 2011

What is the best framework for delivering forefront computational capabilities to a broad user community – researchers and students?

What should be the future of nuclear data from theory?

Suggestions

This is an “Emerging Need for Nuclear Data”

May best be served by a partnership of existing nuclear data efforts with a team of nuclear theorists and computer scientists

Feedback? - - - Questions?

Toward conceptualizing the path forward:

What are the needs – user communities to be served?
Investors, stakeholders, developers, users, . . .

Is there an existing set of applicable “best practices”?

What are the next steps?

Sample options for computational environments to consider/evaluate

- Potential Workflow environment – high end/ provenance
- Data Base Management System
- Nuclear Physics Calculator – Extreme single particle shell model
- Nuclear Physics Calculator – MFDn (see demo)